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Surface states and annihilation characteristics of positrons trapped at the (100) and (111) surfaces of silicon [57]

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Abstract

Recent studies of Si(100) and Si(111) using positron annihilation induced Auger-electron spectroscopy (PAES) reveal that experimental annihilation probabilities of surface trapped positrons with relevant Si core-level electrons differ significantly for two faces of clean Si, an elemental semiconductor. These experimental results are investigated theoretically by performing calculations of the "image-potential" positron surface states and annihilation characteristics of the surface trapped positrons with relevant Si core-level electrons for the ideally terminated, nonreconstructed and reconstructed Si(100)-(2 X 1) and Si(111)-(7 X 7) surfaces. Computed positron surface binding energies demonstrate their sensitivity to the specific atomic structure of the topmost layers of surfaces, and, when compared to positron work functions, the stability of positron surface states on all studied Si(100) and Si(111) surfaces. The positron surface state wave function was found to be localized in a potential well on the vacuum side at both nonreconstructed semiconductor surfaces. The (2 X 1) reconstruction of the Si(100) surface causes the positron surface state wave function to extend into the lattice in the regions where atoms are displaced away from their ideal terminated positions. A comparison of theoretical and experimental positron surface binding energies for Si(100) shows that the best agreement is achieved when the reconstructed Si(100)-(2 X 1) surface is described within the asymmetric dimer model. Calculations indicate that the positron surface state wave function is localized in all three dimensions in the corner hole regions of the reconstructed Si(111)-(7 X 7) surface. This localization provides an explanation for previous experiments that failed to show the anisotropy in the electron-positron pair momentum density distribution expected for a positron surface state delocalized in the plane of the surface. Positron annihilation characteristics are calculated for each surface and compared with experimental positron spectroscopy data. These calculations reveal strong dependence of positron annihilation characteristics on the crystal face of clean Si in contrast to the much smaller face dependence found on clean metal surfaces. Annihilation probabilities of surface trapped positrons with Si 2s- and 2p-core-level electrons are found to be significantly smaller for the reconstructed Si(111)-(7 X 7) surface when compared with the results for the reconstructed Si(100)-(2 X 1) surface, in agreement with experimental PAES data. These results indicate that PAES intensities, which are proportional to core annihilation probabilities, are sensitive to the crystal face and surface structure of an elemental semiconductor.

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